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X-Division Research Note:

"GENERALIZATION OF BOOTH'S CODE FOR ADAPTIVE MONTE CARLO TRANSPORT"

Abstract

A code ("Code") had been written by Tom Booth (XTM), which enabled him to test his algorithms for adaptive Monte Carlo transport. The subject effort generalized the Code to enable testing for potential false learning (FL) situations. The generalization allows specifying multiple spatial domains (*i.e.*, line-intervals, spanning multiple mean-free-paths [mfp]), for the so-called "tri-directional problem."

This effort was accomplished in two distinct stages. The first stage involved recasting the Code into a modular form, which enabled the author to follow the logic of the original more easily. The second stage involved the actual generalization to multiple intervals, along with some niceties such as references to Booth's X-Division research note that presents the theoretical basis for the Code's algorithms.

1. Introduction

This Research Note describes an effort to generalize a Fortran code ("Code"), originally written by Tom Booth (XTM). Tom wrote the original code to test his algorithms for continuous (on a line) adaptive Monte Carlo transport.[1, 2] The goal of the subject effort was to enable testing of Tom's theory for potential false learning (FL) situations.[3] Tom's theory incorporates some "insurance against FL," based on the recognition that, although the global solution is unknown, local behavior *is* known. This "insurance policy" is summarized in Tom's theory by:[2]

$$N'(x) \leq N(x)(\sigma - \sigma_s f) - [\sigma - \sigma_s]\delta \tag{61}$$

and

$$-L'(x) \leq L(x)(\sigma - \sigma_s f) - [\sigma - \sigma_s]\delta \tag{62}$$

If the conditions of Eqs. 61 and 62 are required everywhere, then unbounded weight multiplications are precluded,[2] and "seemed to eliminate most of the FL problems." Testing for FL would necessitate the transport to cover more than a mean-free-path [mfp] on the line, which was the approximate limitation of the original coding.

As is frequently the case, the modification of someone else's code, especially one that was not intended for "production" usage, is a learning process. Stylistic and other differences tend to obscure the underlying logic, so that a preliminary development stage involved a recasting of the original for the sake of clarity (to the code developer). The "real" work of this effort followed the preliminary stage, which, however, was the more labor-intensive stage.

2. Preliminary Stage of Development

In order to recast the original Code for my own comprehension, and avoid introducing bugs in the process, I established a benchmark calculation using the original Code. The output of the benchmark served to monitor my incremental changes, such that each change was accomplished with some degree of confidence that I had not introduced any bugs. Thus, I insisted on "tracking" the benchmark results so long as my changes were only stylistic, and without any changes that would impact the random number sequence. At one point of this recasting process, I did finally make a change that impacted the random number sequence. The results of the benchmark, although they no longer tracked the original digit-for-digit, did converge to the same values within the computed statistical error estimates. This then became my new benchmark for all the subsequent incremental changes.

This preliminary stage was completed via 51 incremental changes, beginning with the original Code. The resulting Code was modular and more amenable to the generalization of the Code that followed. As is my custom, every incremental change was preserved for future reference, by bundling the source code with its computed benchmark (and related information) and archived on the common file system (CFS). At any time, if it becomes necessary to review any step in this development, my archived "documentation" would make that straightforward.

3. Generalization Stage of Development

Once the preliminary stage was accomplished, the Code (and my own comprehension of its logic) was ready for generalization to transport on a line, having arbitrary length [mfp], comprising an arbitrary number of segments. The latter is important, because Tom's algorithms for the Taylor-series expansion of the importance function becomes "strained" for excessively long expansion [mfp]. The Code computes the importance on the section (*i.e.*, line-segment) boundaries, and uses Taylor expansion elsewhere. Thus, even the use of a Taylor expansion with 50 terms (or any finite number of terms) has a limited range of applicability.

The relevant equations in Tom's theory are:[2]

$$N(x) = \sum_{i=0}^{\infty} N^{(i)}(x)\Big|_{x=y} \frac{(x-y)^i}{i!} \tag{67}$$

$$L(x) = \sum_{i=0}^{\infty} L^{(i)}(x)\Big|_{x=y} \frac{(x-y)^i}{i!} \tag{68}$$

where the forward and backward importances, $N(y)$ and $L(y)$, respectively, are known at some particular section boundary y, and $N^{(i)}(x)$, $L^{(i)}(x)$ are the $i-th$ derivatives at point x. Moreover, Tom derives the equations that relate *all* orders of derivatives at a point in his equations 63–66,[2] which I will not repeat here.

Once the generalization to multiple intervals [mfp] was accomplished, Tom helped me debug the resulting Code. As he himself has reported in the past,[2] debugging any Monte Carlo code is challenging, and the adaptive nature of this Code makes debugging even more challenging.

In this process, we discovered that the "distance-to-collision" sampling necessitates careful adherence to basing the sampling on computed/inferred importances that are continuous over the sampled "distance-to-collision." The continuity of the importance function is preserved only within each line-segment interval (by virtue of the expansion algorithm), and so the sampling had to be modified from its original algorithm. The original took advantage of the fact that the importance estimates were originally made on *one boundary only*, and the expansion thereby guaranteed continuity over the whole length of the line, albeit for only about 1 [mfp]. The new sampling algorithm performs stepwise sampling over the intervals, until it is determined that a collision within a specific interval occurs (or the history terminates in capture/reflection/transmission).

4. Results

Using the generalized Code, Table I below shows a comparison of results for a 1 [mfp] line, using a Taylor series of order 50, and 10 iterations of 5000 particles per iteration. Scattering was assigned equal probability in both directions (forward/backward).

TABLE I
Results for 2-, 4-, 8-Segments Compared with Theory
(computed relative error for mean in parentheses)

	Computed Forward-Importance on Boundary				
# B	Source/Reflection	$\frac{1}{4}$ point	Mid-point	$\frac{3}{4}$ point	Transmission
3	0.4820037 (4E-8)		0.6969846		1.0
5	0.4820037 (4E-8)	0.5804017	0.6969846	0.8354051	1.0
9	0.4820037 (4E-8)	0.5804017	0.6969846	0.8354051	1.0
Theory	0.48200365 ...	0.58040172 ...	0.69698462 ...	0.83540508 ...	1.0

The theoretical result was computed by a code based on the analytic solution.[4]
B *means* total number of boundaries.

5. Summary

Adaptive Monte Carlo transport relies on learned information to accelerate convergence to a zero-variance biasing solution. Such an iterative procedure may be vulnerable to false learning (FL). Any scheme that attempts to avoid such FL must also avoid precluding zero-variance biasing. The latter may occur if the scheme is too conservative in it's treatment for undersampled domains of phase space. Hence, a delicate balance between the requisite convergence rate and the all-important correct result must be struck.

As reported by Tom,[2] he has incorporated in the Code a procedure that may preclude FL. I have also reported[3] some evidence that the *tendency* to inspect all states has the *tendency* to avoid FL. And we have identified a potential basis for diagnosing the presence of FL, namely, a comparison between theoretical and computed values of quantities related to local behavior.[2, 3] Such comparisons are based on the recognition that, although the global solution is unknown, local behavior *is* known.

As a result of the subject effort, the efficacy of Tom's "insurance against FL" can now be investigated. For convenience, the current generalized version of the Code is maintained on the WWWeb.[5]

REFERENCES

[1] T. E. Booth, "Tridirectional Problem Discretization for LDRD,"
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[4] Tom Booth, private communication.

[5] H. Lichtenstein, "Generalized Code Source Listing,"
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